

Table I. Crystallographic Data and Refinement Statistics

| Data Collection | GRASP55 1-208 |
|--|----------------------------------|
| Space group | P4 ₁ 2 ₁ 2 |
| Unit cell dimensions (Å) | a = b = 88.0 c = 61.2 |
| Resolution (Å) | 62.25-1.65 |
| Outer shell (Å) | 1.68-1.65 |
| Number of reflections | |
| unique | 26,966 |
| total | 356,291 |
| Mean I/ σ (I) | 57.9 (2.40) |
| Completeness (%) | 96.0 (75.8) |
| R _{sym} (%) | 5.0 (52.4) |
| Refinement | |
| R factor/R _{free} ^{b,c} | 17.6/22.2 |
| Nonhydrogen atoms | |
| Total | 1877 |
| Solvent | 252 |
| Rmsd from ideal geometry | |
| Bond lengths (Å) | 0.026 |
| Bond angles (°) | 2.11 |
| Average isotropic B values (Å ²) | 24.4 |
| Ramachandran plot | |
| Most favorable region (%) | 84.5 |
| Additional allowed region (%) | 14.3 |
| Generous allowed region (%) | 0.0 |
| Disallowed region (%) | 1.2 |

Values in parenthesis correspond to those in the outer resolution shell.

^aR_{sym} = (| Σ I - \langle I \rangle |)/(Σ I), where \langle I \rangle is the average intensity of multiple measurements.

^bR factor = $\Sigma_{hkl} ||F_{obs}(hkl)| - |F_{calc}(hkl)|| / \Sigma_{hkl} |F_{obs}(hkl)|$.

^cR_{free} = the cross validation of R factor for 5% of reflections against which the model was not refined.